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Estimated Theoretical Models for Optical Constants for CuO_2 doped Polystyrene films

Mahasin F. Hadi Al-Kadhemy&Rana IsmaelKhaleel

Al-Mustansiriya Univ.- College of Science- Physics Dept.

Baghdad/ IRAQ

Corresponding author: drmahasinf@yahoo.com, drmahasinf@gmail.com

Abstract

An analysis study for optical constants of PS-CuO_2 thin films has been studied. The effect of doping percentage of CuO_2 to polystyrene films onthe optical properties concluded from absorption and transmission measurements by using UV-VIS absorption spectrophotometer in the wavelength range (200-900nm).The refractive index (n), and extinction coefficient (k) have been evaluated experimentally and theoretically. Theoretical equation for refractive index (n) is:-

$$y = \frac{(a+cx)}{(1+bx)}$$

And estimated theoretical equation for extinction coefficient (k) is:-

$$y = (a + cx^{0.5})/(1 + bx^{0.5})$$

This was achieved by making fitting curves for all practical data using [Table curve 2D, version 5.01] program.This helps us to estimate a good similar data between experimental and theoretical results, and estimate any data that is not taken experimentally.

Key words: Optical Constants, Polystyrene Polymer, $CuO_{2,}$ Theoretical Model,Effect of Doping Percentage.

1- Introduction

Plastic compounds are present in many target designs for inertial confinement fusion to achieve high gain. Moreover, experiments on fundamental processes such as hydrodynamic instabilities studies, have involved plastic as a basic material [1].In recent years, polymers with different optical properties have been attracted much attentions due to their applications in the sensors[2],light-emitting diodes and others[3].The optical properties of these materials can be easily tuned by controlling constants fordifferent concentrations.

The addition of conductive fillers to the polymer giving a new product called as conducting polymer composite materials (CPCM)which consist of a random distribution of conducting throughout an insulating polymer [4]. The purpose of use of fillers can be divided into two basic categories: - first, to improve the properties of materials and second, to reduce the cost of component [5].

The polymer used in this work is polystyrene. It is a perfect polymer for optical measurements [6], and immunological assays and soluble in aromatic hydrocarbon solvents, cyclohexane and chlorinated hydrocarbons.

Polystyrene is vinyl polymer[7],structurally, it is a long hydrocarbon chain, with a phenyl group attached to every other carbon atom is produced by free radical vinyl polymerization as shown in fig.(1)[8]:-

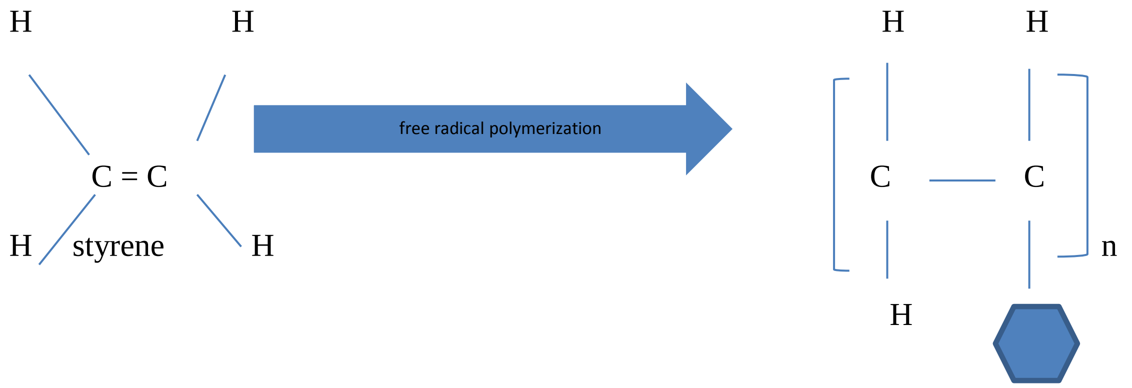

Fig. (1) Chemical structure of polystyrene[8].

Polystyrene, like other polymers, contains a very simple molecular structure [8], yet still exhibits many very interesting physical properties. For example, many scientists are still studying the radiation-induced reactions of polystyrene, as they show very complicated reactions despite their simple structures.

The optical behaviors of materials are utilized to determine their optical constants (refractive index (n), and extinction coefficient(k)).Several methods were proposed to determine the optical constants;they involve spectra photometric measurements of sample in the wavelength range[9].

The extinction coefficient (imaginary part of the refractive index) can be calculated by the relation[10]:-

$$K = \frac{\alpha\lambda}{4\pi} \qquad (1)$$

Where (λ) is the wavelength, (α) is the absorption coefficient which can be obtained using the following equation [11]:-

$$\alpha = \frac{2.3 \log\frac{1}{T}}{x} \qquad (2)$$

Where(T) is the transmittance.

(x) is the thickness of the sample.

The refractive index (n) can be measured (when the reflectance (R) and (K) are Known) by using the equation [12]:-

$$n = \sqrt{\frac{4R(R+1)}{(R-1)^2 - K^2(R-1)}} \qquad (3)$$

The optical study gives information about the fundamental properties of materials under investigation [13].Analysis of the absorption spectra in the lower energy part gives information about atomic vibration while the higher energy part of the spectrum gives knowledge about the electronic states in theatom[14].So thatin the present work, we are study the effect of additive on the optical properties of glassy polymer. The polymer used is polystyrene (PS) with additives (CuO_2) in different concentrations. Also, we estimated theoretical models for this effect on two optical constants; the refractive index (n) and the extinction coefficient (K).

2- Experimental work

Polystyrene (PS), supplied by (ICI) company in the form of granules were used as matrix. Chloroform of purity 99.99 was used as a solvent. A dopant (Cu_2O) was supplied by (Al-Sawari) company.

(PS) grains of weight (0.2) gm were dissolved in (5) ml of chloroform to obtain solution of 4%wt. /wt. The solution was shaken very well by hand for (1/2) hour or more to obtain homogenous mixture. Then, the mixture was cast into a glass sheet of dimensions ($5 \times 5cm^2$) and kept in a dry atmosphere at (40˚C) for (24) hours. The dried films were then removed easily using tweezers clamp.

The chosen concentrations of dopants relative to pure (PS) in (wt. /wt.) were (0.02, 0.04 and 0.06); the measurements of absorbance and transmittance spectra in the wavelength range (200-900nm) were carried out using UV/160/Shimadzu Spectrophotometer.

3- Results and Discussion

Our results involve experimental part and theoretical part as follow:-

3-1 Experimental part

The refractive index (n) of pure and doped PS with CuO_2 were determined using eq.(3).Fig.(1) shows variation of (n) as a function of wavelength(λ),this figure showed that the(n) of doped PS increases with increasing (λ)on the other hand (n) showed a systematic increase with increasing(CuO_2) concentration[15].

The dependence of extinction coefficient (K) on the wavelength obtained using eq.(1)is shown in Fig.(2) for pure and doped samples. It is noticed that (K)value of pure sample has reduced becomes smaller at the region near the absorption edge, and becomes very small with increasing (λ). While(K) for doped sample with (CuO_2) shows an increase with increasing (λ). The maximum peaks belong to maximum absorption of (CuO_2).Where(K) shows an increase with increasing doping concentration(0.02,0.04,0.06)wt.%.The behavior of (K) can be indicates that dopant atoms of (CuO_2)will modify the structure of the host polymer[16].

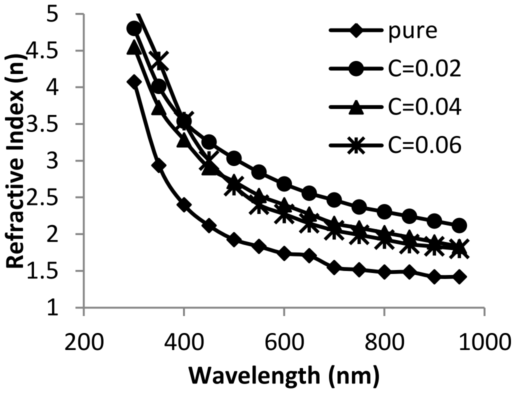

Fig.(2)Variation in refractive index(n) as function of wavelength of pure and doped PS.

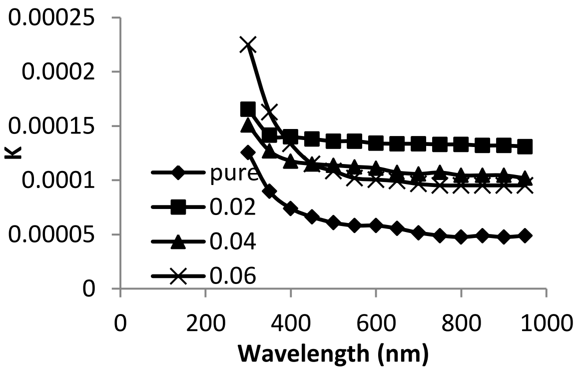

Fig.(3) Variation in extinction coefficient (K) as function of wavelength of pure and doped PS.

3-2Theoretical Part

3-2-1 Estimate Theoretical Model for Refractive Index

In Order to facility to estimate theoretical model for the effect of concentration of CuO_2 doped PS and pure PS on the refractive index constant of optical properties, first we make a fitting curve to the relation between refractive index and wavelength for pure PS as shown in Fig.(4),and then we make a fitting curve to the relation between refractive index and wavelength for CuO_2 (0.02) doped PS as shown in Fig.(5),and for CuO_2(0.04) doped PS as shown in Fig.(6),and for CuO_2(0.06)doped PS as shown in Fig.(7).

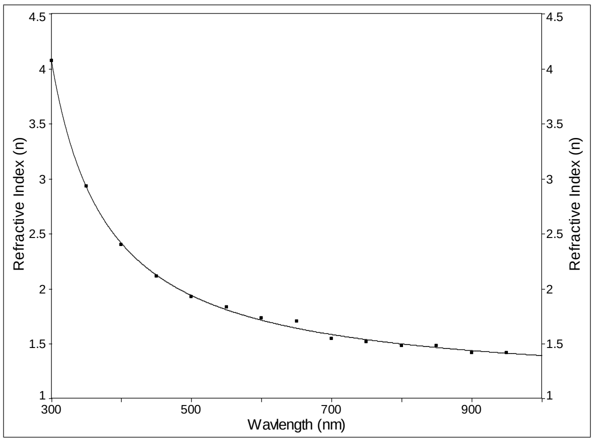

Fig.(4) Fitting curve of the relation between refractive index and wavelength for pure PS

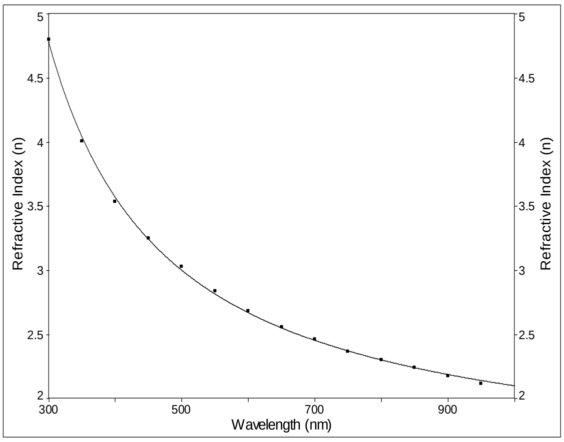

Fig.(5) Fitting curve of the relation between refractive index and wavelength for C=0.02 of CuO_2 doped PS

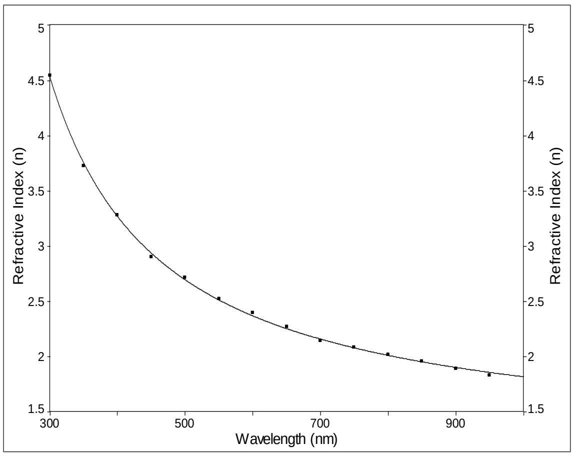

Fig.(6) Fitting curve of the relation between refractive index and wavelength for C=0.04 of CuO_2 doped PS

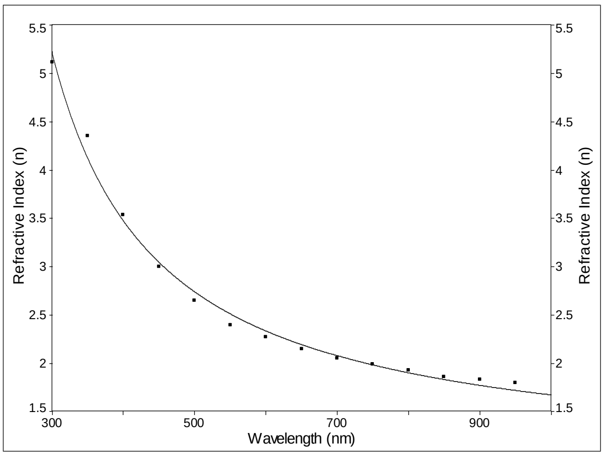

Fig.(7) Fitting curve of the relation between refractive index and wavelength for C=0.06 of CuO_2 doped PS

The best estimated theoretical equation is:-

$$y = \frac{(a+cx)}{(1+bx)} \quad (4)$$

Where x and y act wavelength and refractive index, respectively.And a_1, b_1, and $c_1$describe parameters of equation which varied with concentration of CuO_2 , and the value of these parameters illustrate in table (1).

Table (1)

The parameters of fitting equation for (n) constant for pure PS and different concentration of CuO_2

Parameter	Pure PS	C=0.02	C=0.04	C=0.06
r^2	0.9988594599	0.9992872051	0.9993451737	0.9921811624
a_1	0.013619435	-3.45099035	-2.91623152	-3.10090992
b_1	-0.00452821	-0.00815927	-0.00739439	-0.00646628
c_1	-0.00493321	-0.01159357	-0.00872303	-0.00604506

Where r^2 acts the correlation factor between experimental and theoretical data.
The a_1, b1 and c_1 parameters plotted against concentration of CuO_2 as shown in figs. (8-10), respectively. The fitting equations of these figures are written above each figure.

$$y_1 = \frac{(0.011214469 - 798089.84x_1^2)}{(1 + 251864.3x_1^2)} y_2 = 0.17338662 - 0.049892527x_1^{0.5}$$

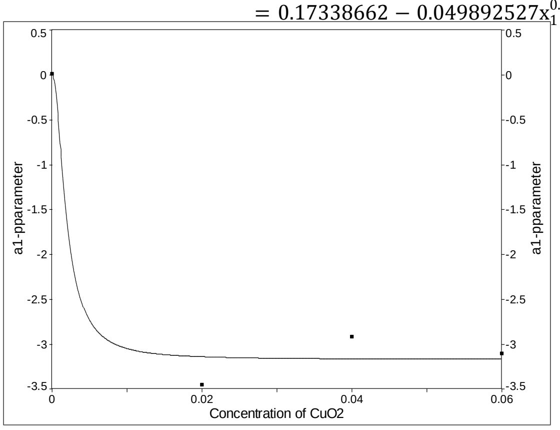

Fig.(8) The relation between concentration of CuO_2 and a_1-parameter.

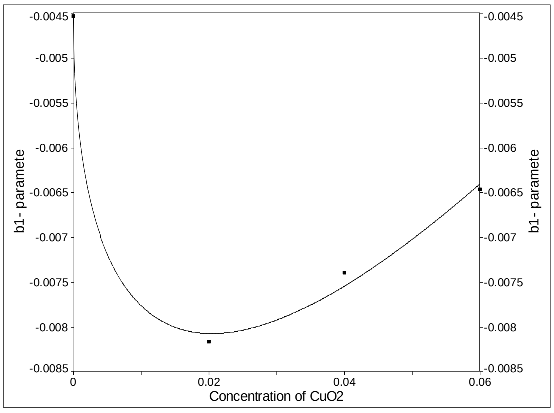

Fig.(9) The relation between concentration of CuO_2 and b_1-parameter.

$$y_3 = -7062.9181 + 1785.0308x_1\hat{}0.5 + 6860.0933e\hat{}(-x_1)$$

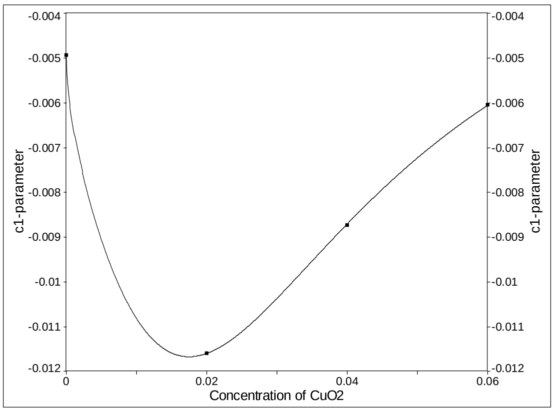

Fig.(10) The relation between concentration of CuO_2 and c_1-parameter.

Where y_1,y_2 and $y_3$in fitting equations represent a_1,b_1 and c_1 parameters, respectively, and x_1 represent the concentration of CuO_2. We choose test concentration CuO_2 as C=0.03 to prove our model.

The estimated theoretical equation for test concentration of CuO_2 C=0.03 is:-

$$y = \frac{(-3.1547623-0.010374005x)}{(1-0.0079216x)} \quad (5)$$

Then plotted this test concentration with experimental curves, as in fig.(11).this is a good matching between the behavior of these curves(experimental and theoretical).

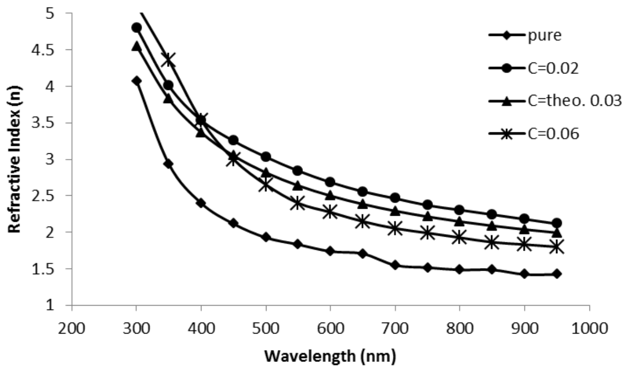

Fig.(11) Theoretical and experimental relation between refractive index and wavelength for pure PS and different concentration of CuO_2 doped PS.

3-2-2 Estimate Theoretical Model for Extinction Coefficient

In Order to facility to estimate theoretical model for the effect of concentration of CuO_2 doped PS and Pure PS on the extinction coefficient (K) constant of optical properties; fig. (3). First we make a fitting curve to the relation between extinction coefficient and wavelength for pure PS as shown in Fig(12),and then we make a fitting curve to the relation between extinction coefficient and wavelength for CuO_2 (0.02) doped PS as shown in Fig.(13),and for CuO_2(0.04) doped PS as shown in Fig(14),and for CuO_2(0.06)doped PS as shown in Fig(15).

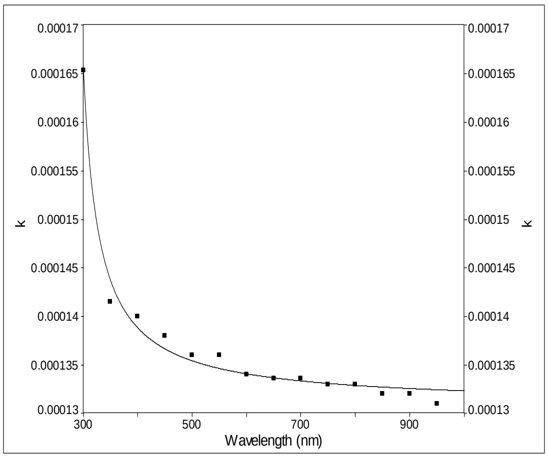

Fig.(12) Fitting curve of the relation Between extinction coefficient and wavelength for pure PS.

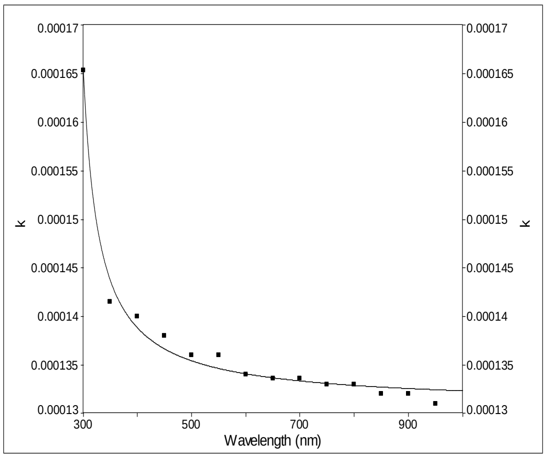

Fig.(13)Fitting curve of the relation betweenrefractive index and wavelength for C=0.02 of CuO_2 doped PS

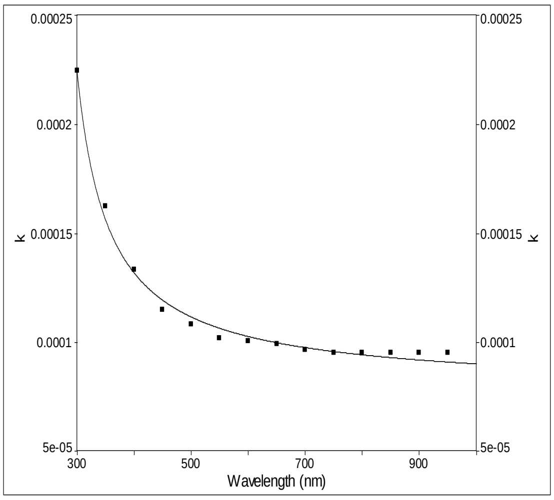

Fig. (14) Fitting curve of the relation between extinction coefficient and wavelength for C=0.04 of CuO_2 doped PS.

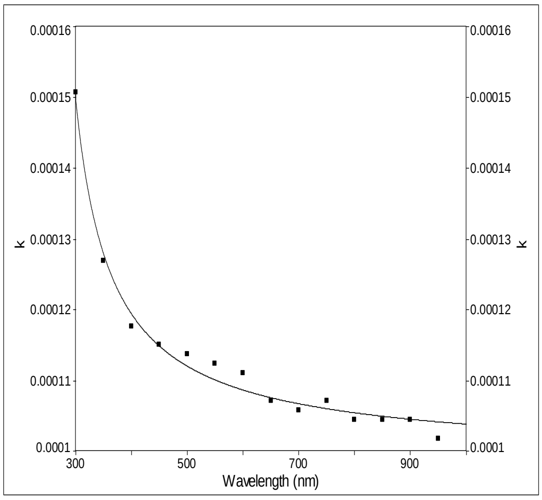

Fig. (15) Fitting curve of the relation between extinction coefficient and wavelength for C=0.06 of CuO_2 doped PS.

The estimated theoretical equation is:-

$$y_4 = (a_2+c_2x^{0.5}) / (1+b_2x^{0.5}) \qquad (6)$$

Where $y_4$representextinction coefficient K and x act wavelength λ. The value of $a_{2,}$ $b_{2,}$ and c_2 parameters illustrate in table (2).

Table (2)

The parameters of fitting equation for pure PS for different concentration of CuO_2

Parameter	Pure PS	C=0.02	C=0.04	C=0.06
r^2	0.99624357	0.98681115	0.98705963	0.99237414
a_2	2.3183429e-6	0.00012858181	9.1272919 e-5	5.8869836 e-5
b_2	-0.065546553	-0.060722186	-0.06479445	-0.063755775
c_2	-2.3205228 e-6	-7.9170928 e-6	-6.3315171 e-6	-4.7601023 e-6

Where r^2 act the correlation factor between experimental and theoretical data, The fitting equation of these figures are written above each figure.

$$y_4 = 4 * 0.000127442\, n(1-n) y_5 = -0.06635617 - \frac{0.05208961}{lnx} - 0.13279786/(lnx_1)^2$$

Where $n = \exp(-\frac{x_1+0.00145884}{0.029603538})$

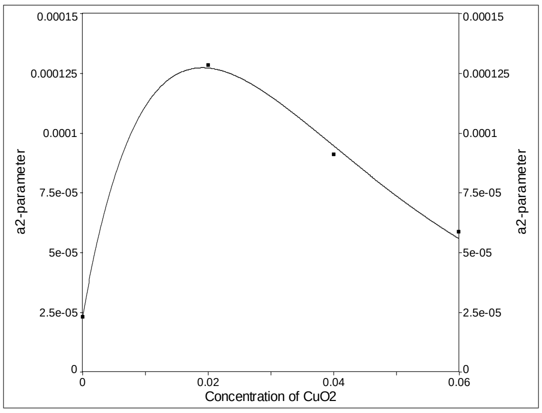

Fig. (16)The relation between concentration of CuO_2 and a-parameter

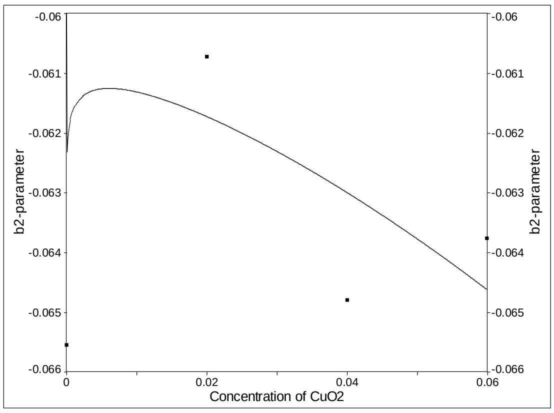

Fig. (17)The relation between concentration of CuO_2 and b-parameter

$$y_6 = -4 * 7.8119e - 6\, n(1-n)$$

Where$n = \exp(-x_1 + 0.00308849)\,/0.036358276$

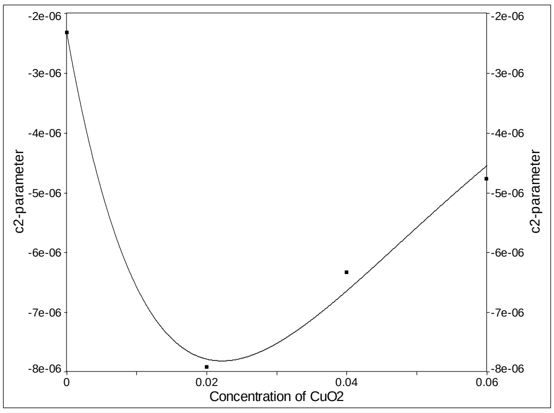

Fig. (18)The relation between concentration of CuO_2 and c-parameter

Two test concentrations of CuO_2, C=0.05 and C=0.08 where chosen to estimate the theoretical model.

The estimated theoretical equation for C=0.05 is:-

$$y_4 = (7.387\mathrm{e}^{-5} - 2.8558\mathrm{e}^{-6}\mathrm{x})^{0.5}/(1 - 0.06655\mathrm{x})^{0.5} \quad (7)$$

And the estimated theoretical equation for C=0.08 is:-

$$\mathrm{y}_4 = (3.046\mathrm{e}^{-5} - 2.8558\mathrm{e}^{-6}\mathrm{x})^{0.5}/(1 - 0.06655\mathrm{x})^{0.5} \quad (8)$$

Then experimental and theoretical curves were plotted in fig.(19). All these curves have the same type in behavior, so that we can plot any data for K coefficient for this material without make it experimentally. This is matched with results obtained by Al-kadhemy[17], Al-Kadhemy et al [18].

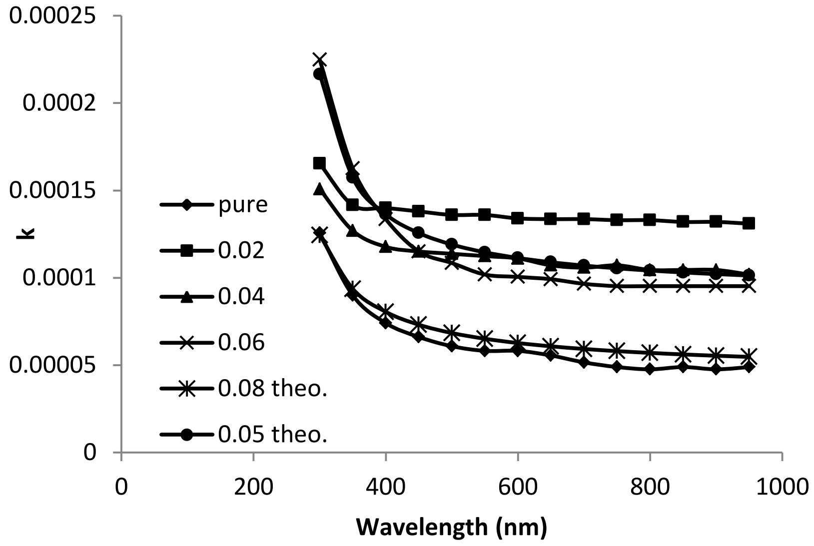

Fig. (19) Theoretical and experimental relation between extinction coefficient and wavelength for pure PS and different concentration of CuO_2 doped PS.

4- Conclusion

The ability of estimating theoretical models from practical data for the effect of doping percentage of CuO_2 to polystyrene films on the optical properties ; refractive index (n) and extinction coefficient (K) was deduced in this work. Very well theoretical results and matched with the behavior of practical results.

5- References

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